

# Multiscale Modelling and Simulation, 15th International Workshop

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**Abstract.** Multiscale Modelling and Simulation (MMS) is a computational approach which relies on multiple models, to be coupled and combined for the purpose of solving a complex scientific problem. Each of these models operates on its own space and time scale, and bridging the scale separation between models in a reliable, robust and accurate manner is one of the main challenges today. The challenges engenders much more than scale bridging alone, as code deployment, error quantification, scientific analysis and performance optimization are key aspects to establishing viable scientific cases for multiscale computing. The aim of the MMS workshop, of which this is the 15th edition, is to encourage and consolidate the progress in this multidisciplinary research field, both in the areas of the scientific applications and the underlying infrastructures that enable these applications. In this preface, we summarize the scope of the workshop and highlight key aspects of this year's submissions.

**Keywords:** multiscale simulation, parallel computing, multiscale computing, multiscale modelling

## 1 Introduction to the workshop

Modelling and simulation of multiscale systems constitutes a grand challenge in computational science, and is widely applied in fields ranging from the physical sciences and engineering to the life science and the socio-economic domain. Most of the real-life systems encompass interactions within and between a wide range of space and time scales, and/or on many separate levels of organization. They require the development of sophisticated models and computational techniques to accurately simulate the diversity and complexity of multiscale problems, and to effectively capture the wide range of relevant phenomena within these simulations.

Additionally, these multiscale models frequently need large scale computing capabilities, solid uncertainty quantification, as well as dedicated software

and services that enable the exploitation of existing and evolving computational ecosystems. Through this workshop we aim to provide a forum for multiscale application developers, framework developers and experts from the distributed infrastructure communities. In doing so we aim to identify and discuss challenges in, and possible solutions for, modelling and simulating multiscale systems, as well as their execution on advanced computational resources and their validation against experimental data.

The series of workshops devoted to multiscale modelling and simulation is organized annually from 2002 [1, 2], and this edition constitutes the 15th occasion that we hold this workshop. The discussed topics cover a range of application domains as well as cross-disciplinary research on multiscale simulation.

The workshop will contain the presentations about theoretical, general concepts of the multiscale computing and those focused on specific use-cases and describing real-life applications of multiscale modelling and simulation.

The first session contains four presentations, geared towards applied mathematics and engineering applications. Vidal-Ferrandiz et al. will present a range of optimization efforts in the context of multiscale modelling of neutron transport, while Olmo-Juan et al. will discuss the modelling of noise propagation in a pressurized water nuclear reactor. Wei Ze et al. will discuss the multi-scale homogenization of pre-treatment rapid and slow filtration processes, both from a computational and an experimental perspective, while Carreno will conclude the session with proposed solutions for the lambda modes problem using block iterative eigensolvers.

The second session contains three presentation, with a focus on medicine and humanity more widely. Garbey et al. will present a flexible hybrid agent-based, particle and partial differential equations method, applied to analyze vascular adaptation in the body. Madrahimov et al., will present results from large-scale network simulations to enable the systematic identification and evaluation of antiviral drugs. Lastly, Groen will present a prototype multiscale migration simulation, which is able to execute in parallel and can be flexibly coupled to microscale models.

Given the nature of the workshop, we look forward to lively discussions as communities from different disciplines will have the opportunity meet and to exchange ideas on general-purpose approaches from different angles. We hope that workshop will help participants to get familiar with the latest multiscale modelling, simulation and computing advances from other fields, and provide new inspiration for their own efforts.

With representation from leading institutions across the globe, the 15th edition of Multiscale Modelling and Simulation Workshop is indeed at the forefront of computational science.

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